



# NSF/ONR Workshop on Data Assimilation in Ocean Research

## LOOPS/Poseidon: A Distributed System for Real-Time Interdisciplinary Ocean Forecasting with Adaptive Modeling and Sampling

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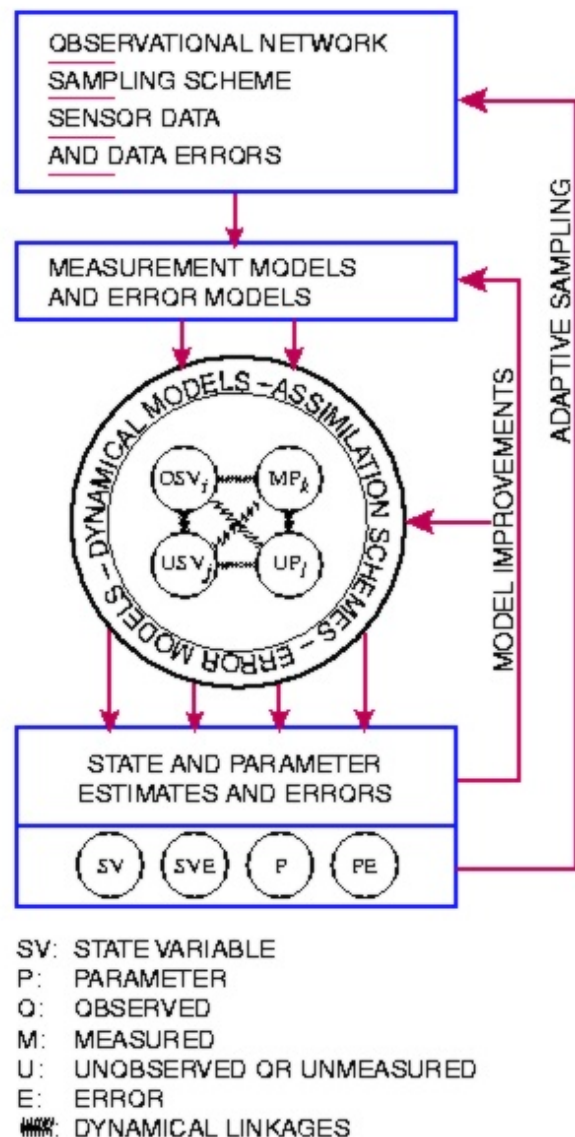
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<http://czms.mit.edu/poseidon>



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# Ocean Science and Data Assimilation



- Field and remote observations
- Models:
  - Dynamical
  - Measurement
  - Error
- Assimilation schemes
- Sampling strategies
- State and parameter estimates
- Uncertainty estimates
- *A Dynamic Data-Driven Application System (DDDAS)*

Fig. 1. Data assimilation system schematic



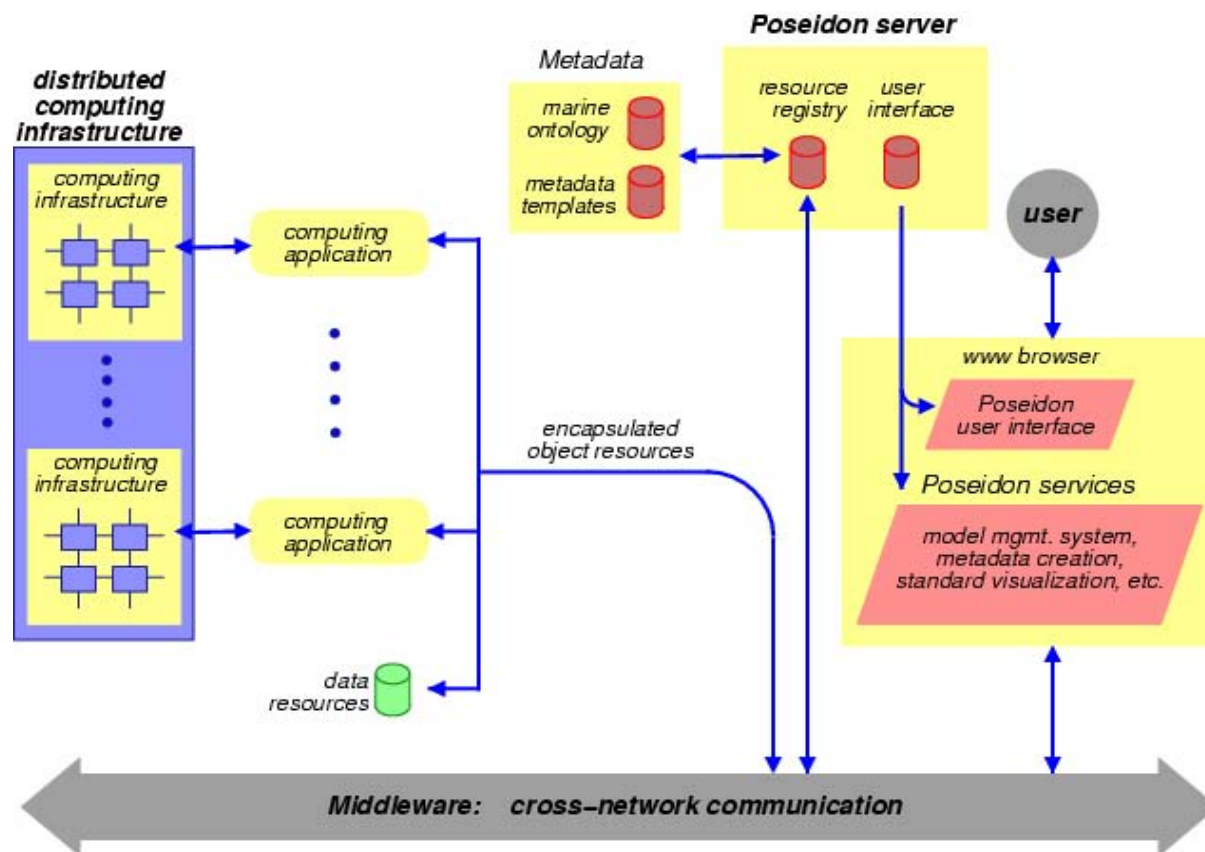
# LOOPS/Poseidon

## Adaptive Interdisciplinary Ocean Forecasting in a Distributed Computing Environment

- Research coupling Physical and Biological Oceanography with Ocean Acoustics.
- More effective Real-Time Ocean Forecasting for Naval and Maritime Operations, Pollution Control, Fisheries Management, Scientific Data Acquisition, etc.
- MIT OE (IT, Acoustics) and Harvard DEAS (Ocean Physics-Biology-Acoustics).

### Key points

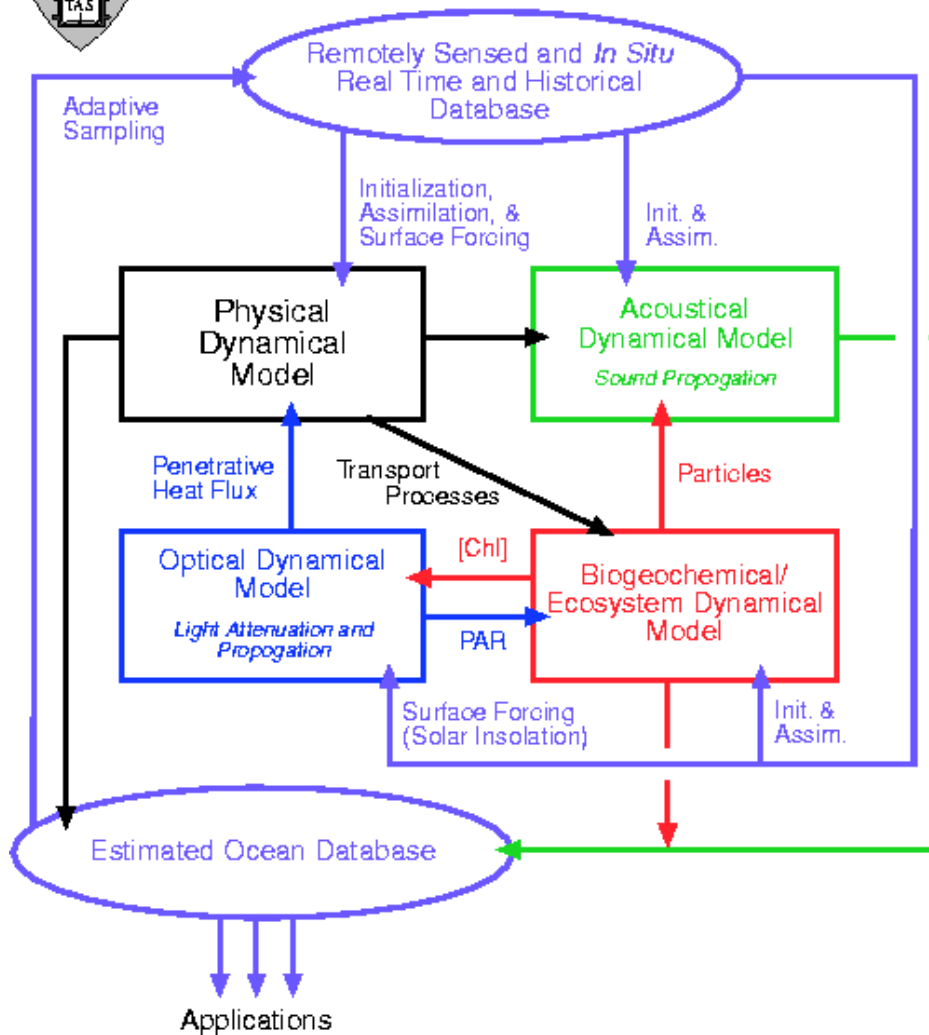
- Web interface
- Remote visualization
- Metadata for code and data
- Metadata/Ontology editors
- Legacy application support
- Grid computing infrastructure
- Transparent data access
- Data assimilation (ESSE, OI)
- Interdisciplinary interactions
- Adaptive modeling
- Adaptive sampling
- Feature Extraction
- Prototype for community-use



# Physical-Biological-Acoustical Oceanography with HOPS

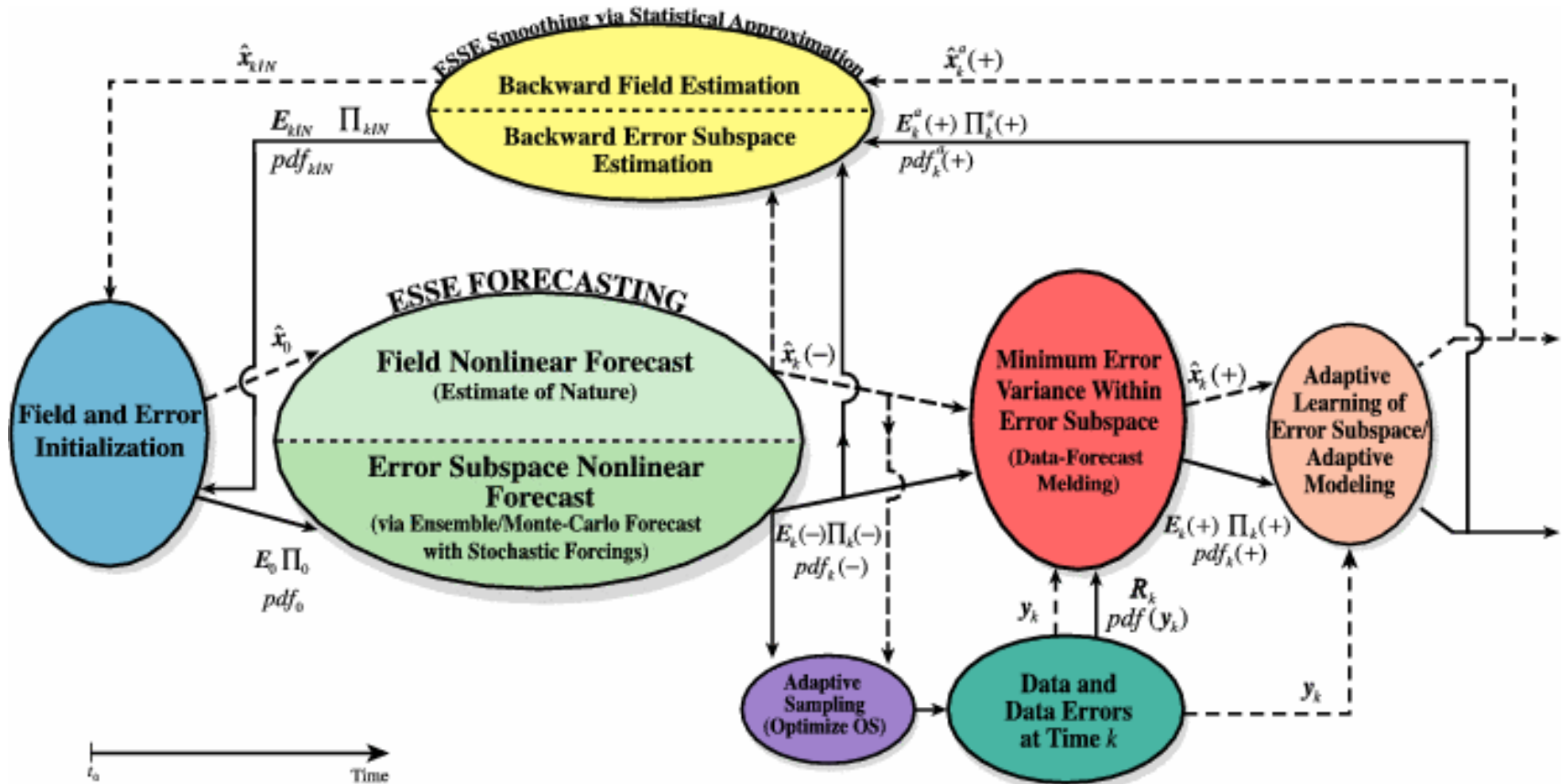


## HARVARD OCEAN PREDICTION SYSTEM - HOPS



- Primitive Equation (PE) physical dynamics model
- Multiple biological models
- Interfaces to acoustical models
- Adaptable to different domains
- Nested-domains parallelism
- Software: F77-matlab-C
- I/O: NetCDF, stdin

# Error Subspace Statistical Estimation (ESSE)



- Uncertainty forecasts (with dynamic error subspace, error learning)
- Ensemble-based (with nonlinear and stochastic model)
- Multivariate, non-homogeneous and non-isotropic DA
- Consistent DA and adaptive sampling schemes
- Software: not tied to any model, but specifics currently tailored to HOPS

# IT Design Motivations

- Real-time predictions of **interdisciplinary** ocean fields and *uncertainties*
  - Data Assimilation (DA) using ESSE is currently ensemble-based and thus ideal for high throughput distributed computing
  - Interdisciplinary interactions and multiscale/nested simulations ideal for parallel computing
- Develop autonomous adaptive models for physics & biology
  - Adaptive parameter values, model structures and state variables
  - Error metrics and criteria for adaptation
- Towards automated, distributed management of observed and modeled data
  - Consistent use of metadata helps provide transparent data management, including quality control
  - Forecasting workflow is being automated, including DA
- Web access from lightweight clients eases operational use and system control
- Interactive visualizations for better understanding and decision-making

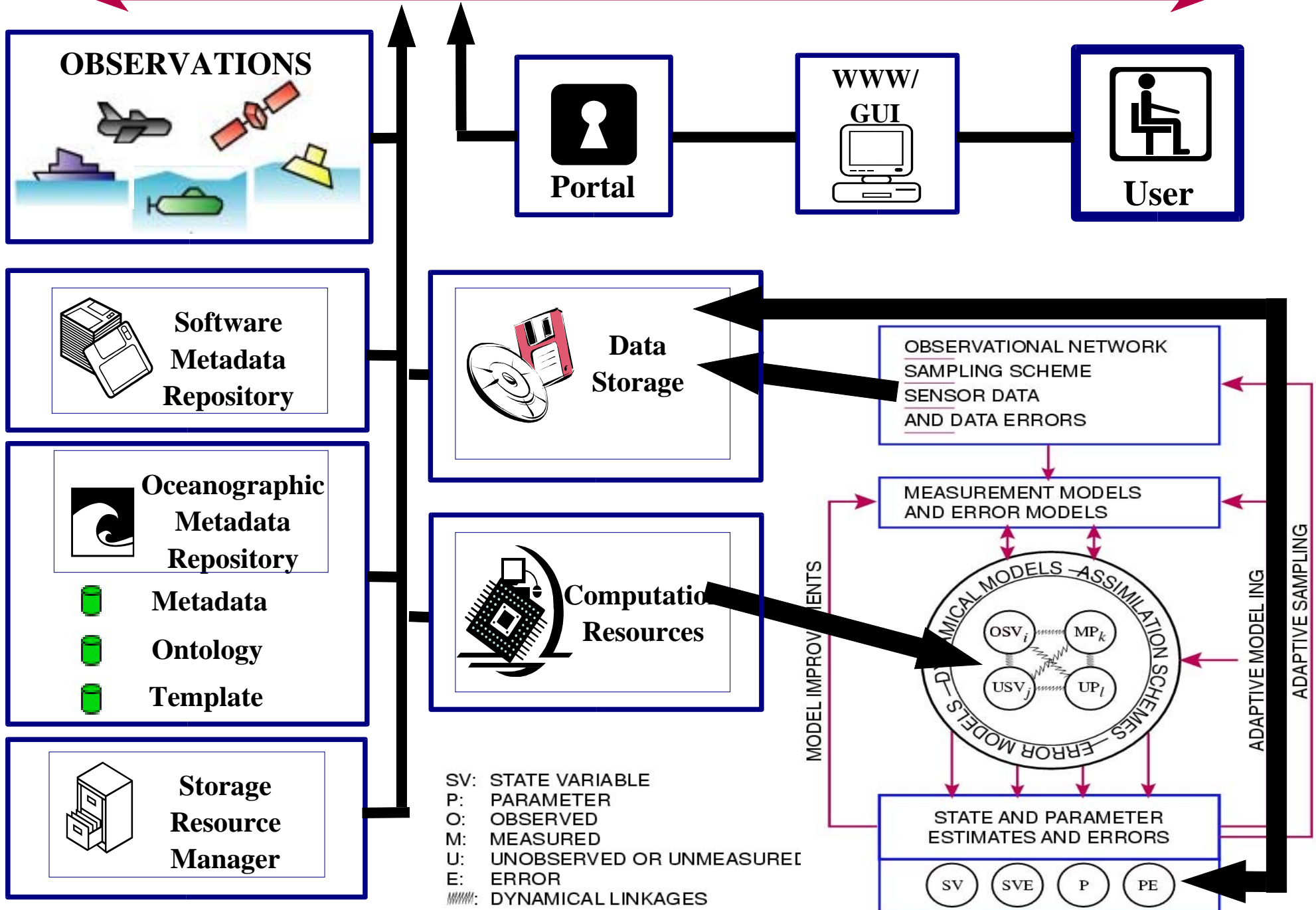


# Software Strategies

- Exploit parallelism (especially throughput) opportunities
- Maximize performance, facilitate users, but limited changes
  - For new generalized adaptive biological model: MPI coding
  - For existing software: automate file I/O based workflows
  - Work to the maximum extent possible at the binary level
  - Metadata for software use (and installation) in XML
- Use Grid technologies
  - For user: compute and data access solutions
  - Drive forecasting, visualization workflows on the Grid
  - Present results to user's web browser



# GRID COMPUTING - MIDDLEWARE

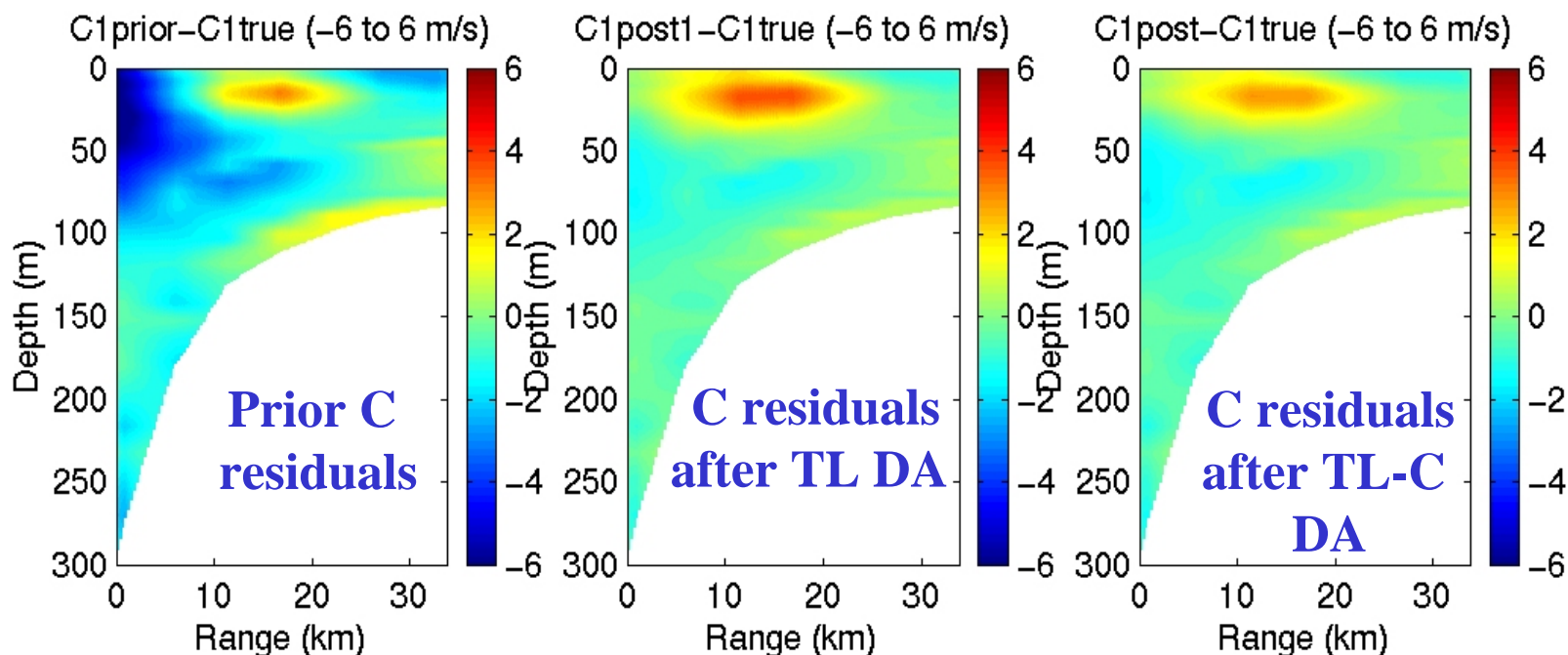


# **Interdisciplinary Data Assimilation (DA)**

- Is in its infancy, but can contribute significantly to understanding physical-acoustical-biogeochemical processes, including quantitative development of fundamental models**
- Required for interdisciplinary ocean field prediction and parameter estimation**
- Model-model, data-data and data-model compatibilities are essential**
- Care must be exercised in understanding, modeling and controlling errors and in performing sensitivity analyses to establish robustness of results**
- Dedicated interdisciplinary research needed**

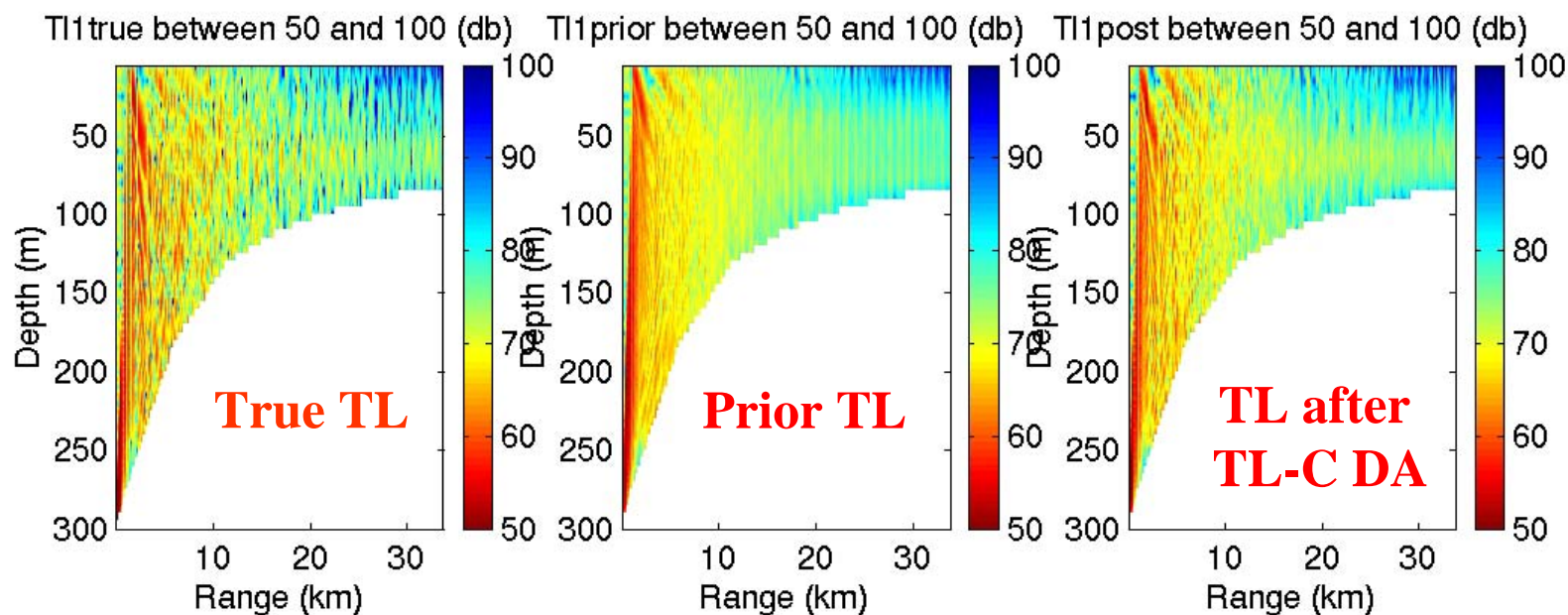
# Coupled Physical-Acoustical Filtering via ESSE

**Coupled  
assimilation of  
sound-speed and  
TL data for a joint  
estimate of sound-  
speed and TL  
fields**

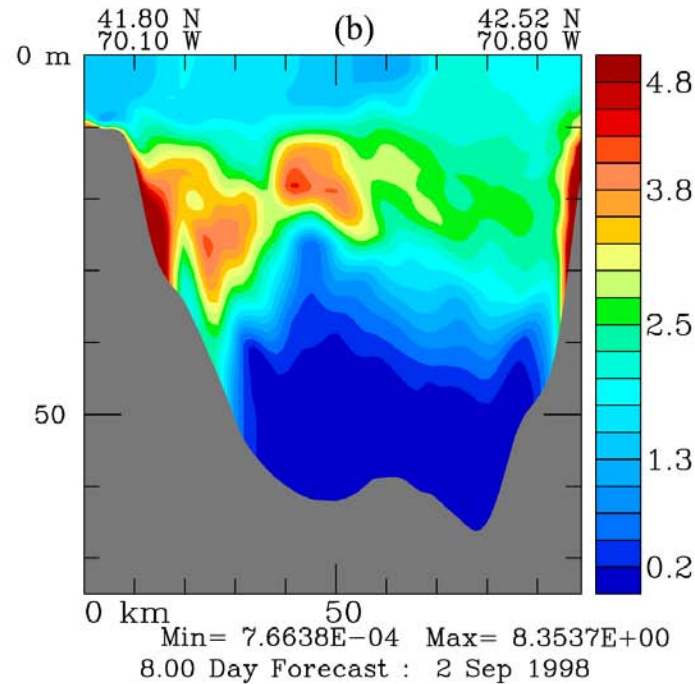
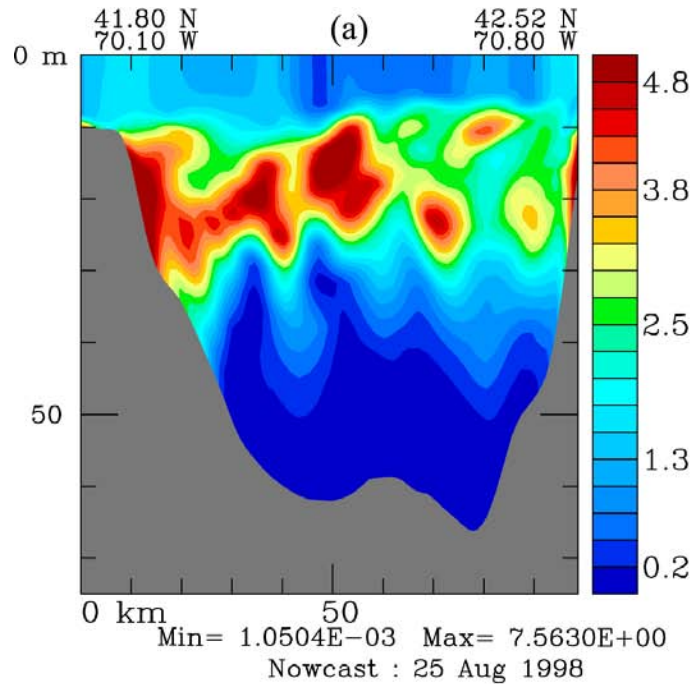


**Twin-experiments:**

- “Truth” ocean physics assimilates natural data
- Provides 3 CTDs
- Corresponding TL “truth” provides towed-receiver TL data, every 500m at 75m depth



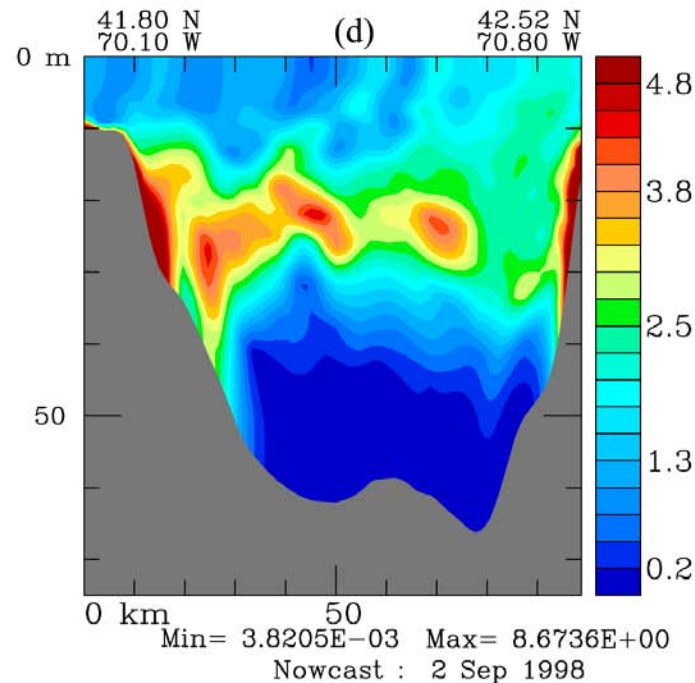
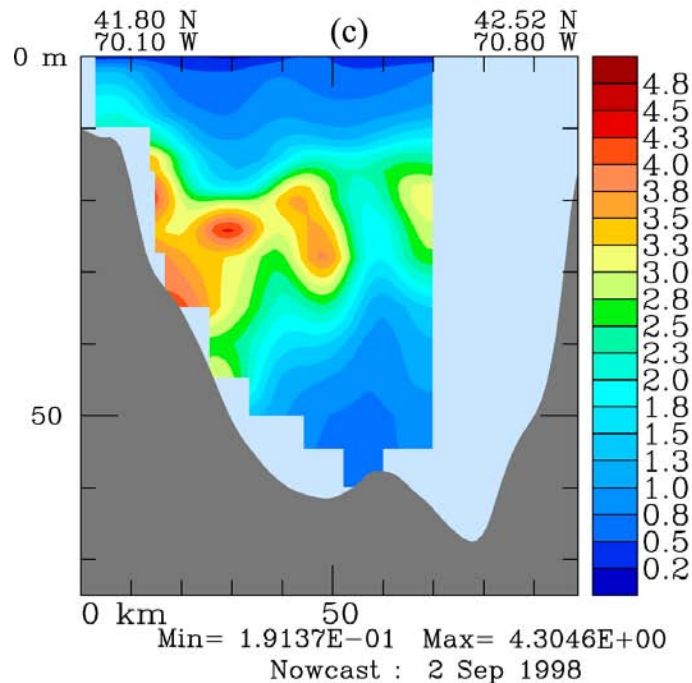
# Coupled Physical-Biogeochemical Smoothing via ESSE



**Cross-sections in Chl-a fields, from south to north along main axis of Massachusetts Bay, with:**

**a) Nowcast on Aug. 25**

**b) Forecast for Sep. 2**

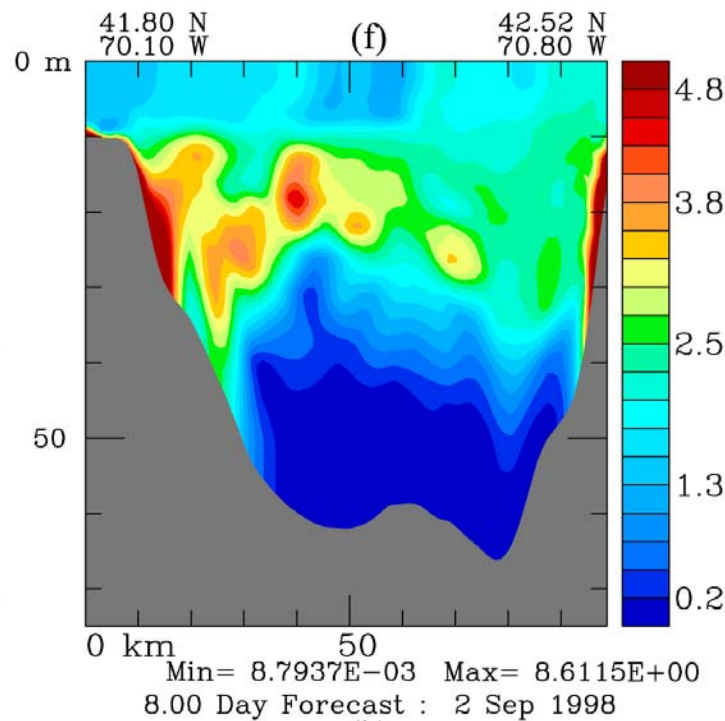
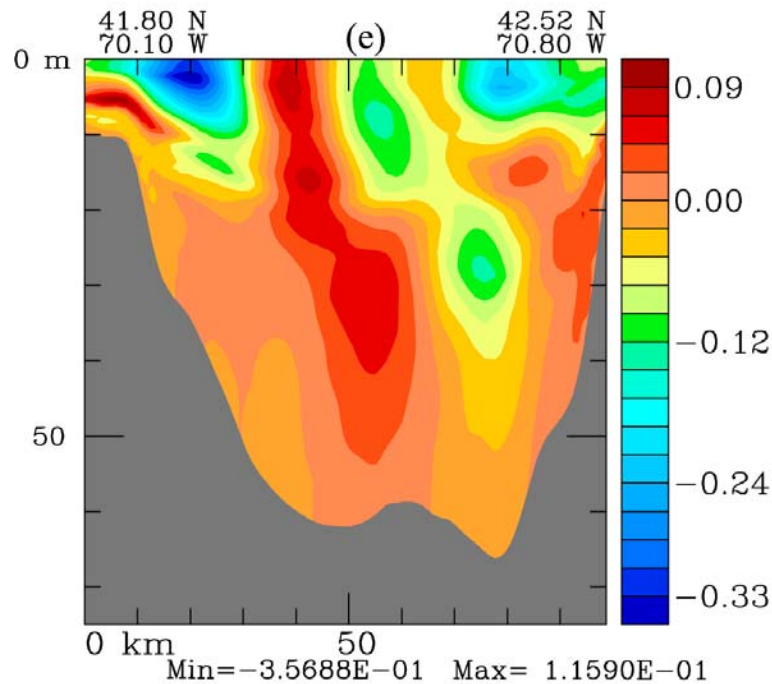


**c) 2D objective analysis for Sep. 2 of Chl-a data collected on Sep. 2–3**

**d) ESSE filtering estimate on Sep. 2**



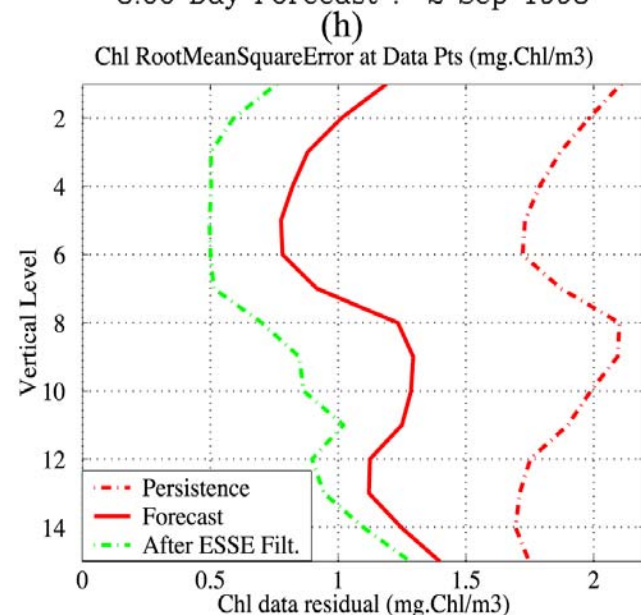
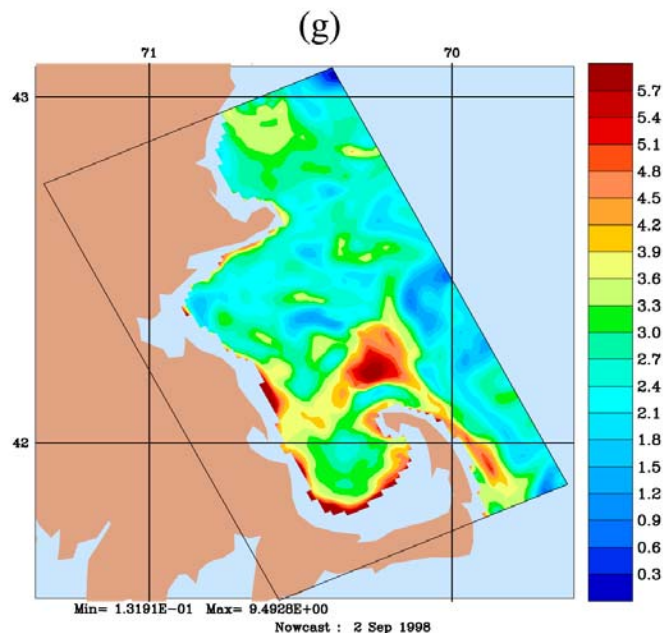
# Coupled Physical-Biogeochemical DA via ESSE (continued)



**e) Difference between ESSE smoothing estimate on Aug. 25 and nowcast on Aug. 25**

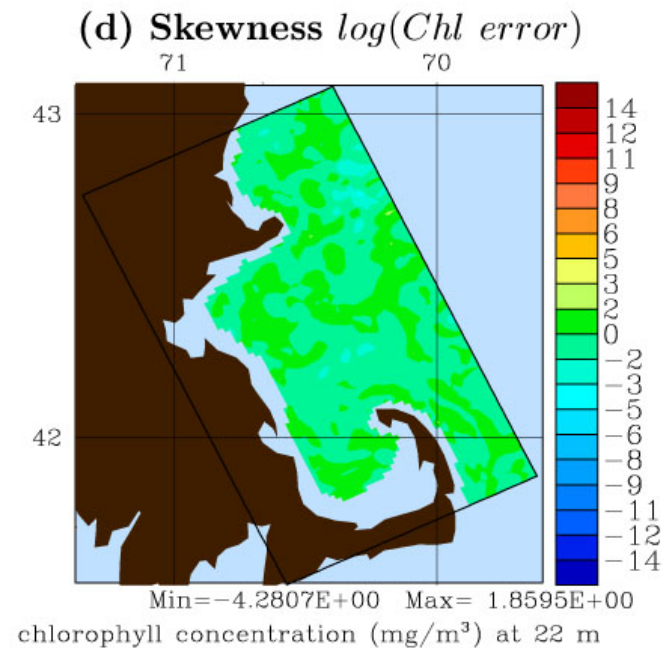
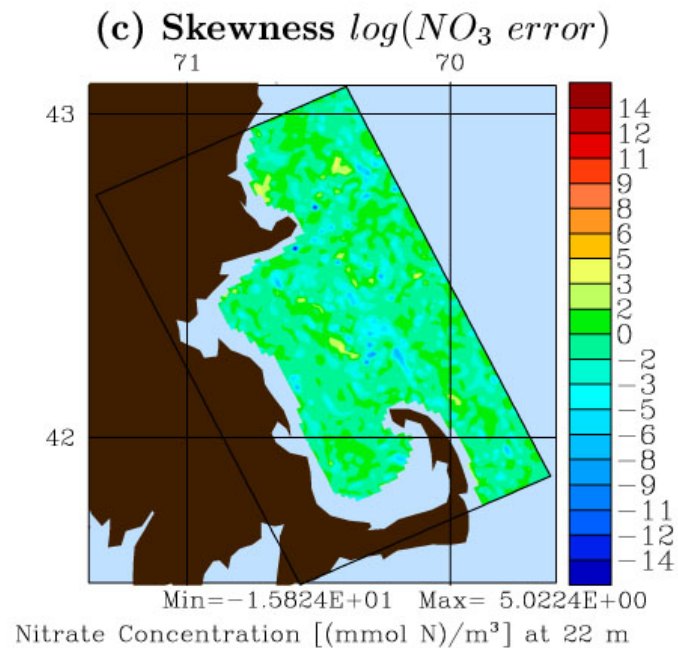
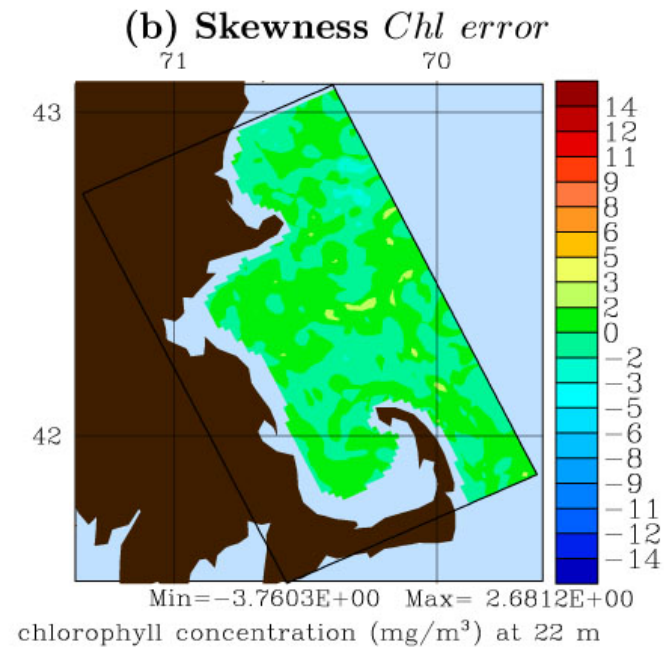
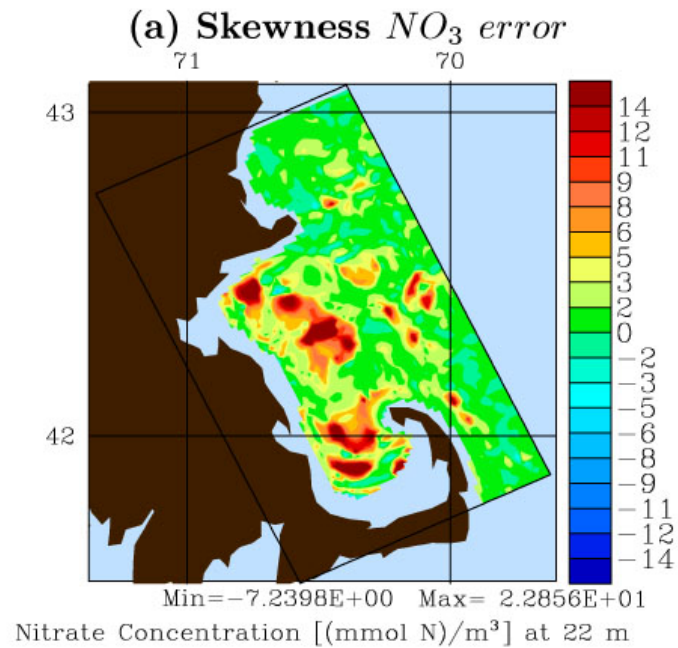
**f) Forecast for Sep. 2, starting from ESSE smoothing estimate on Aug. 25**

**(g): as d), but for Chl-a at 20 m depth**



**(h): RMS differences between Chl-a data on Sep. 2 and the field estimates at these data-points as a function of depth (specifically, “RMS-error” for persistence, dynamical forecast and ESSE filtering estimate)**

# How Gaussian are biogeochemical error forecast distributions?



# Interdisciplinary Adaptive Sampling

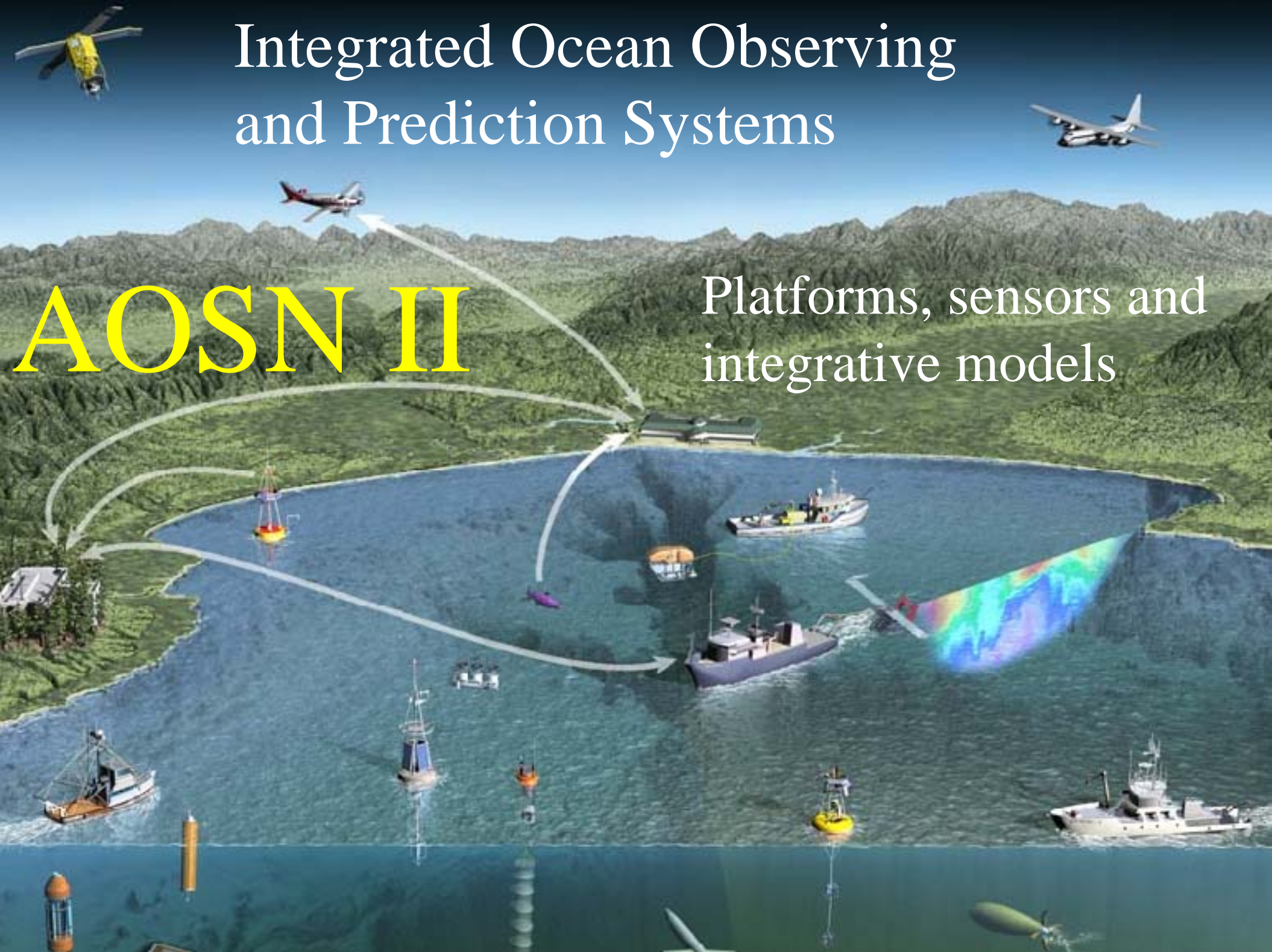
- Use forecasts and their uncertainties to alter the observational system in space (locations/paths) and time (frequencies) for physics, biology and acoustics.
- Locate regions of interest, based on:
  - Uncertainty values (error variance, higher moments, pdf's)
  - Interesting physical/biological/acoustical phenomena (feature extraction, Multi-Scale Energy and Vorticity analysis)
  - Maintain synoptic accuracy
- Plan observations under operational, time and cost constraints to maximize information content (e.g. minimize uncertainty at final time or over the observation period).



# Integrated Ocean Observing and Prediction Systems

## AOSN II

Platforms, sensors and  
integrative models

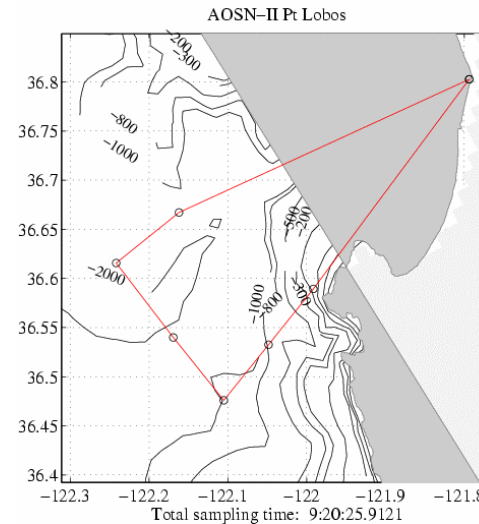


# HOPS/ESSE- AOSN-II Accomplishments

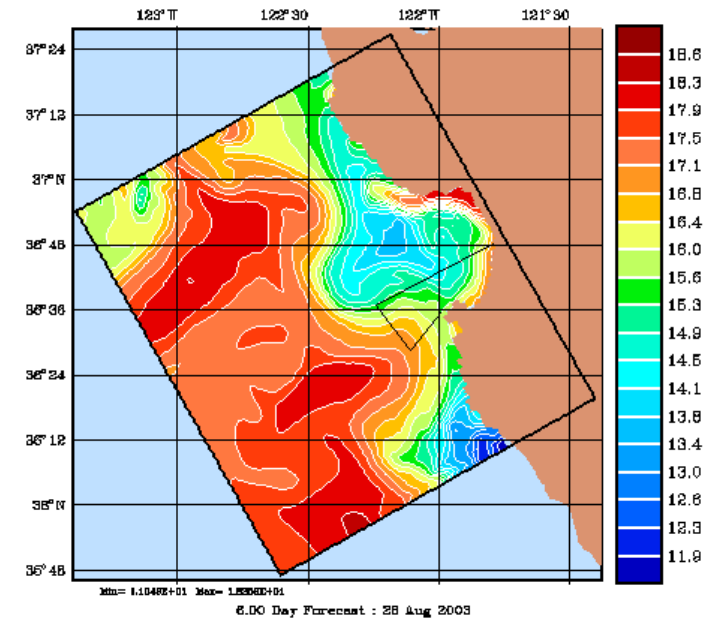
- 23 sets of real-time nowcasts and forecasts of temperature, salinity and velocity released from 4 August to 3 September
- 10 sets of real-time ESSE forecasts issued over same period: total of 4323 ensemble members (stochastic model, BCs and forcings)
- Adaptive sampling recommendations suggested on a routine basis
- Web: <http://www.deas.harvard.edu/~leslie/AOSNII/index.html> for daily distribution of forecasts, scientific analyses, data analyses, special products and control-room presentations
- Assimilated ship (Pt. Sur, Martin, Pt. Lobos), glider (WHOI and Scripps) and aircraft SST data, within 24 hours of appearance on data server (after quality control)
- Forecasts forced by 3km and hourly COAMPS flux predictions

# Real-time Adaptive Sampling – Pt. Lobos

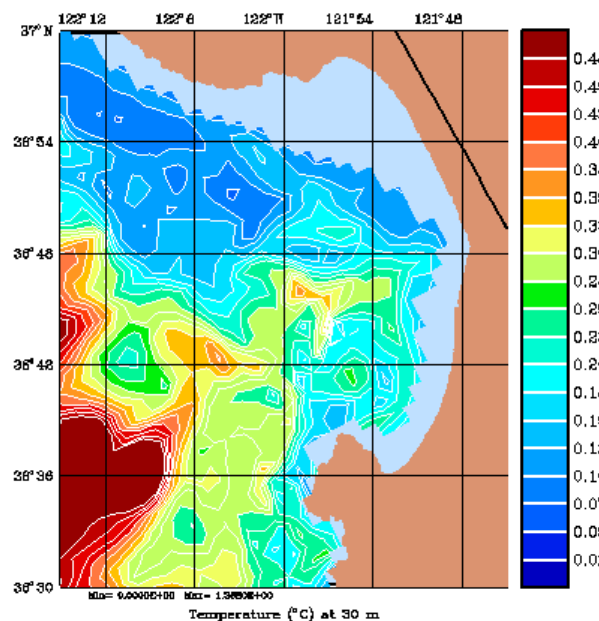
- Large uncertainty forecast on 26 Aug. related to predicted meander of the coastal current which advected warm and fresh waters towards Monterey Bay Peninsula.
- Position and strength of meander were very uncertain (e.g. T and S error St. Dev., based on 450 2-day fcsts).
- Different ensemble members showed that the meander could be very weak (almost not present) or further north than in the central forecast
- Sampling plan designed to investigate position and strength of meander and region of high forecast uncertainty.



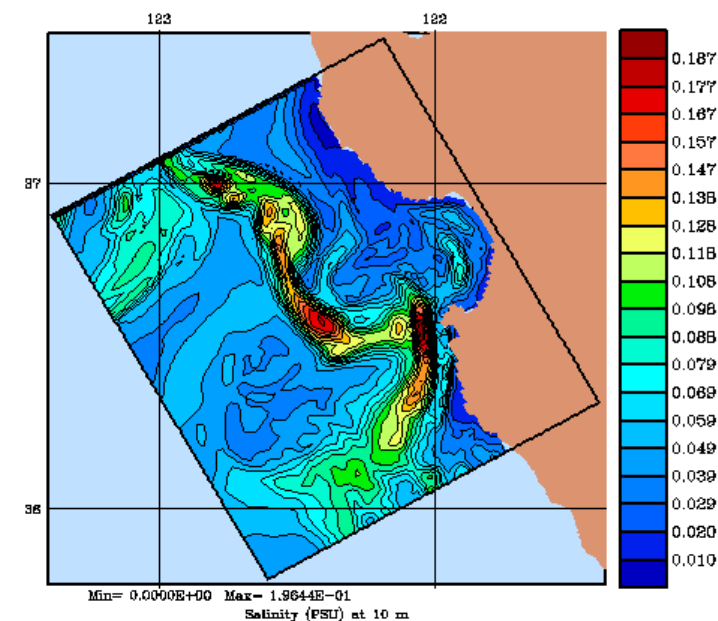
## Surf. Temperature Fct



## Temperature Error Fct

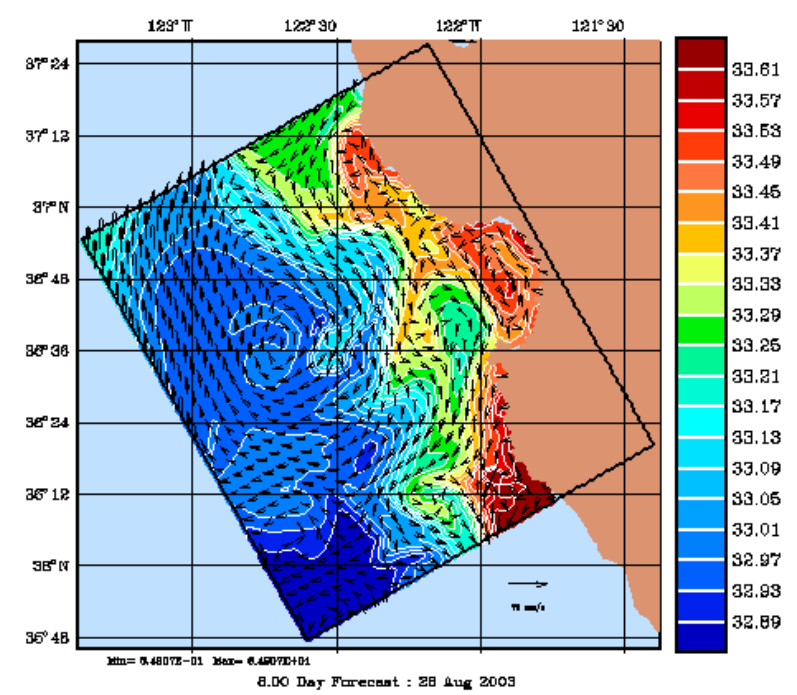
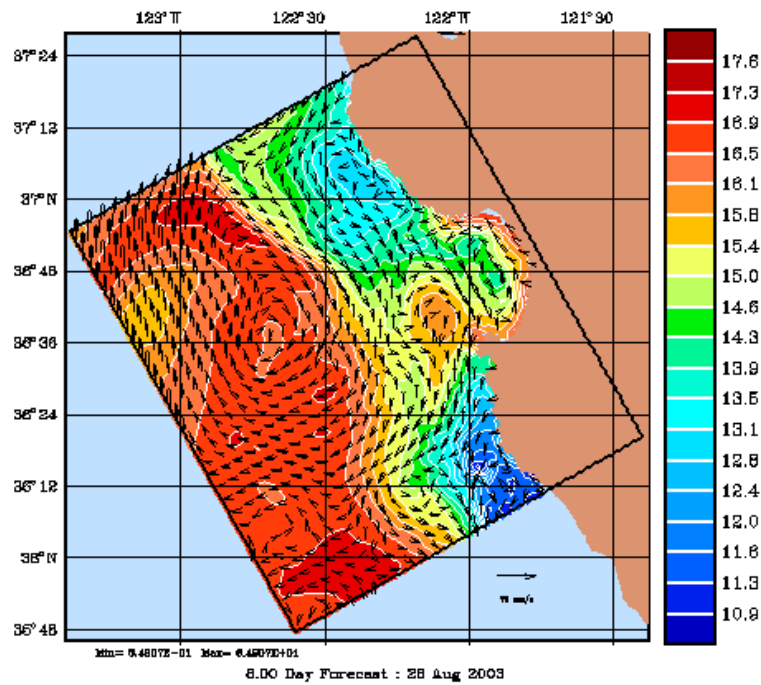


## Salinity Error Fct

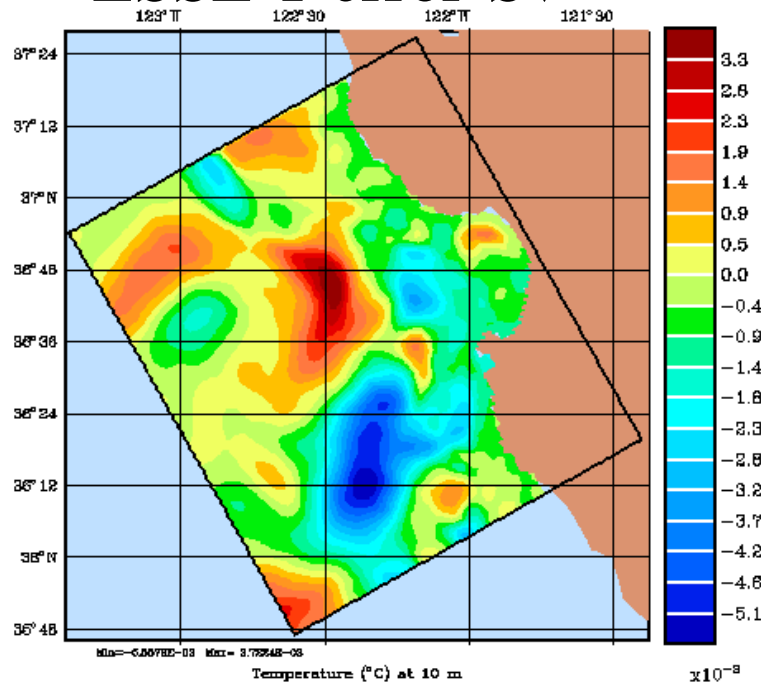




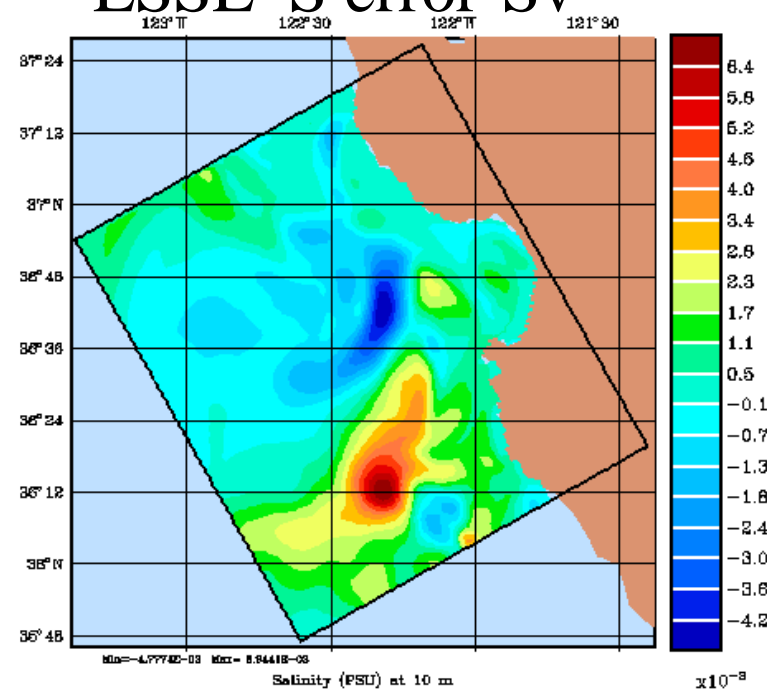
# ESSE field and error modes forecast for August 28 (all at 10m)



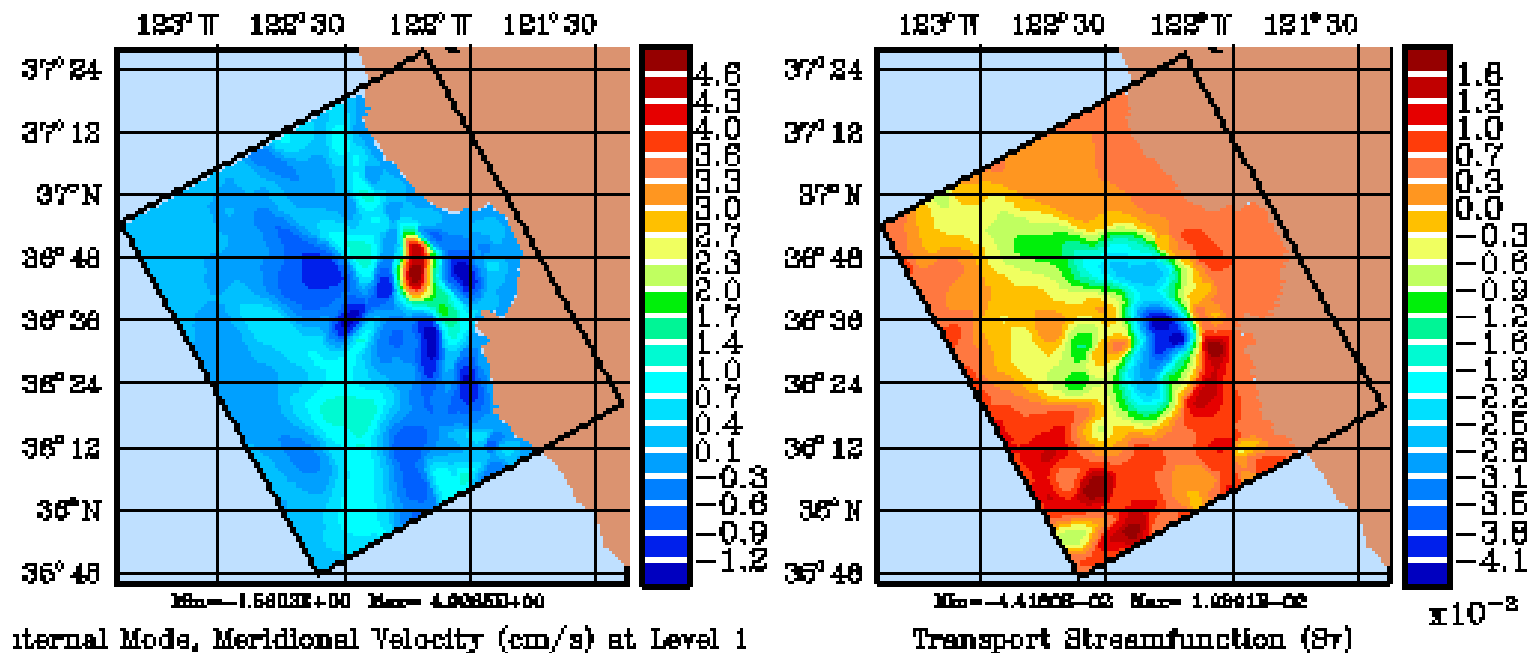
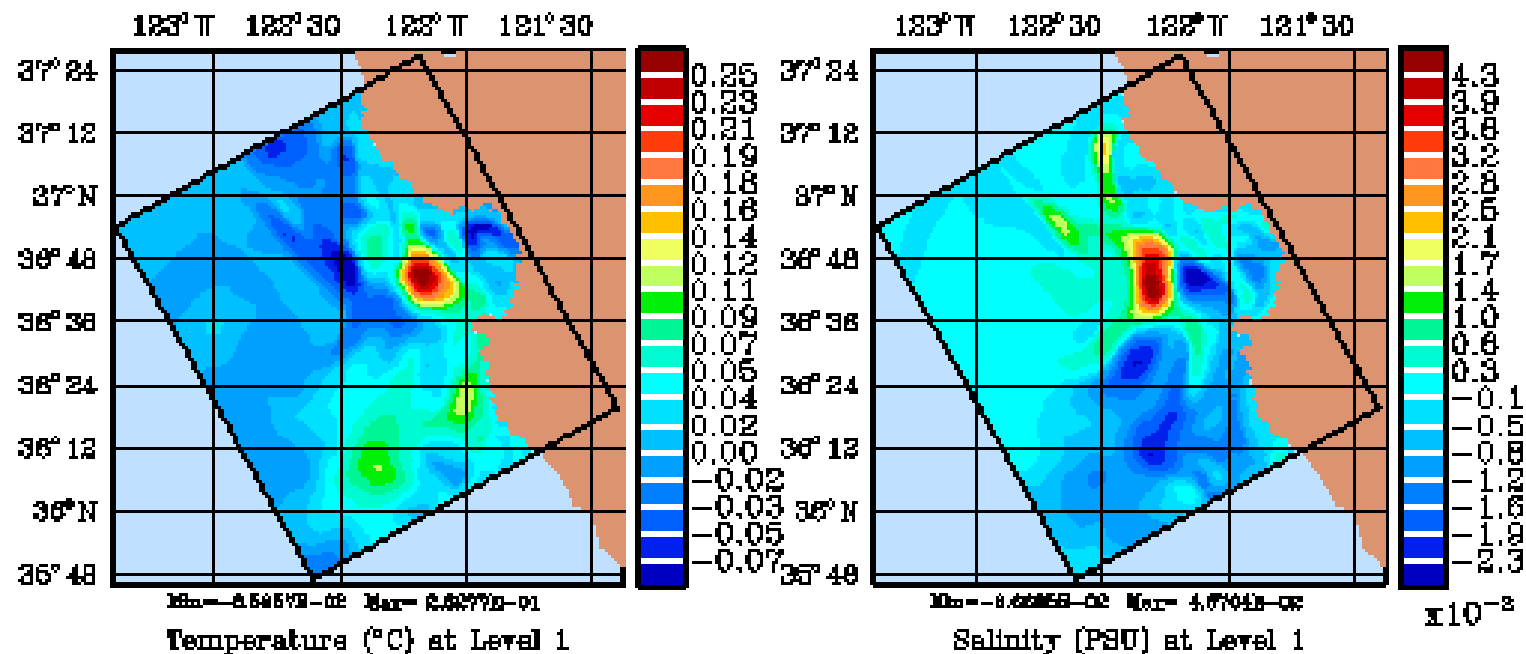
## ESSE T error-Sv



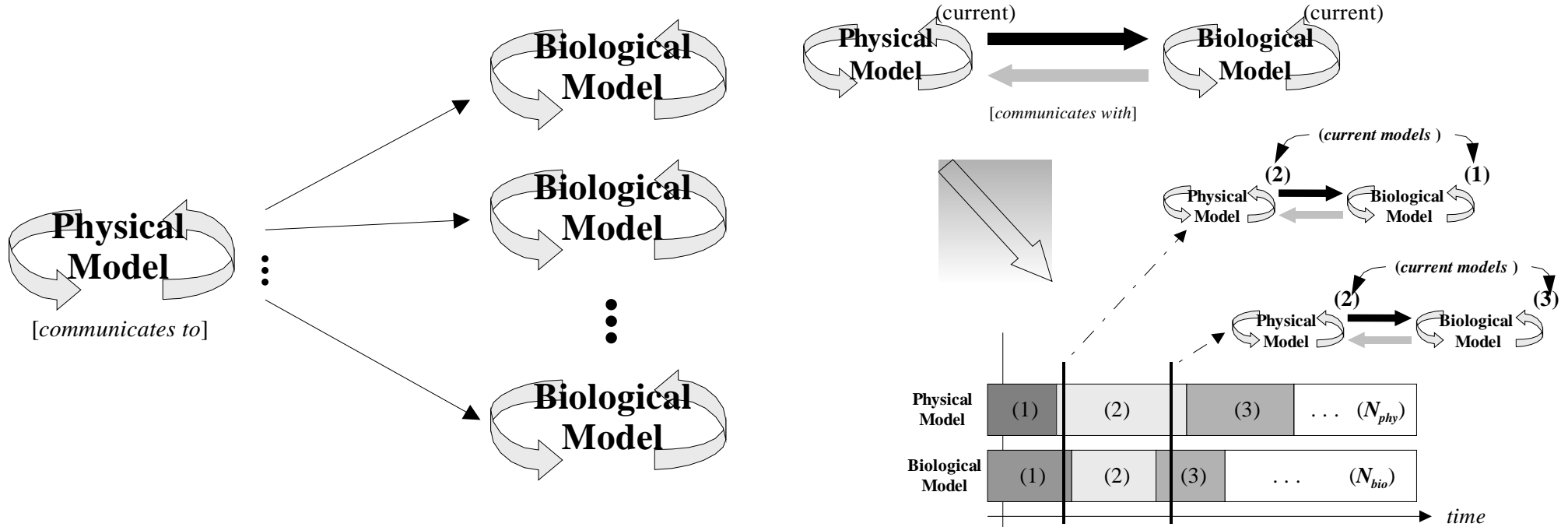
## ESSE S error-Sv



# Error Covariance Forecast for 28 August



# Real-time Adaptive Coupled Models



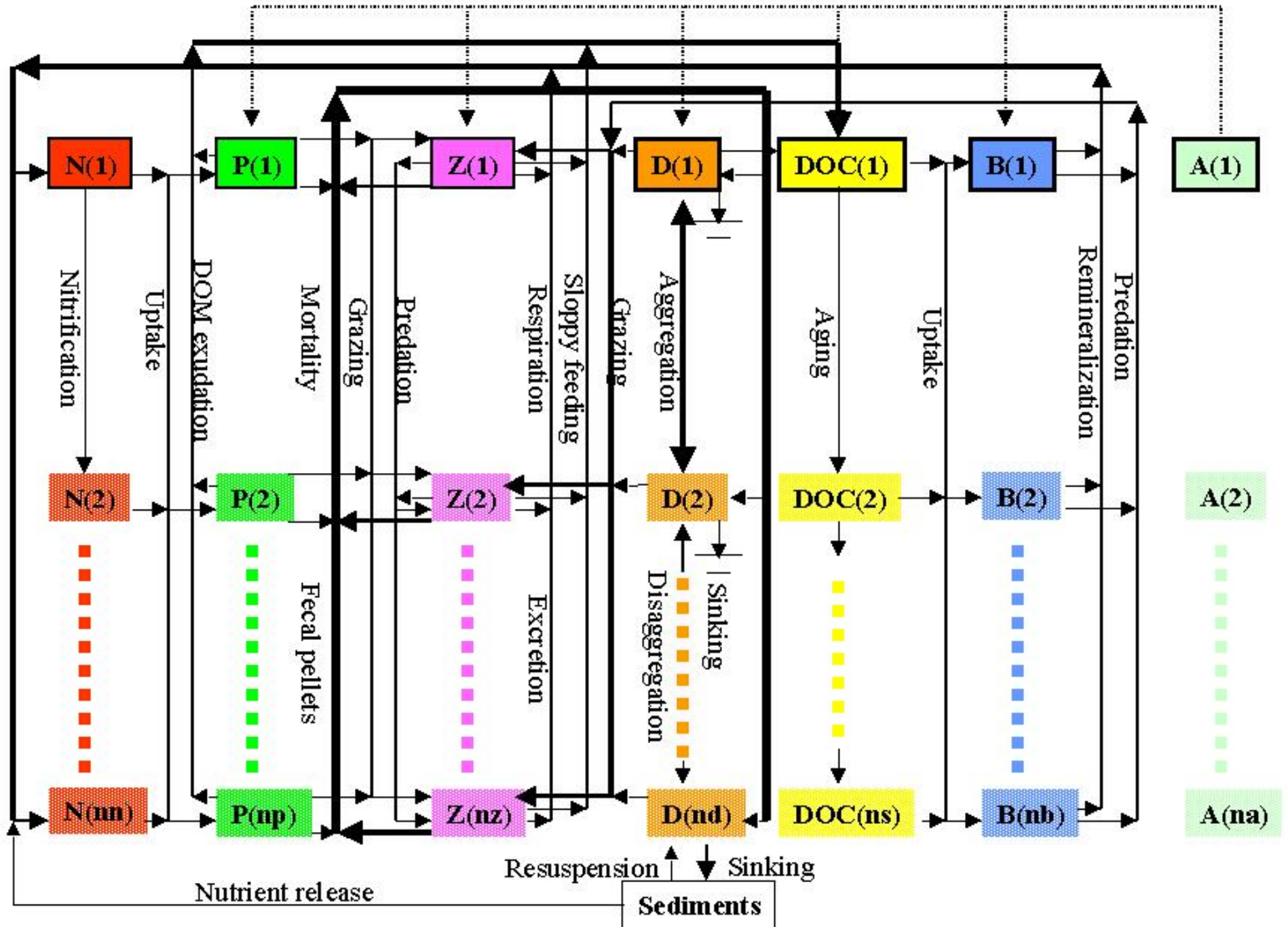
- Different Types of Adaptive Couplings:

- Adaptive physical model drives multiple biological models (biology hypothesis testing)
- Adaptive physical model and adaptive biological model proceed in parallel, with some independent adaptation

- Implementation

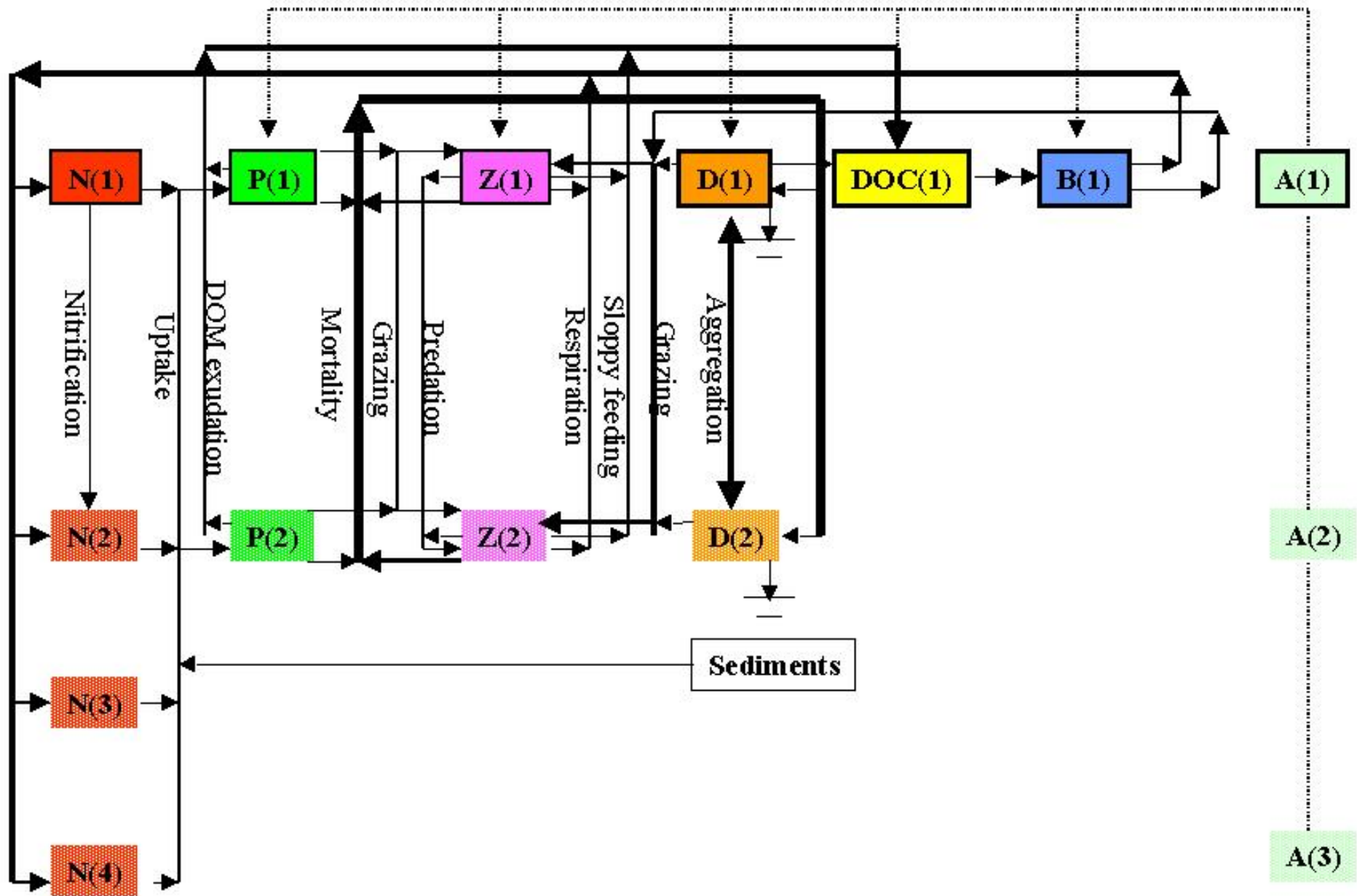
- For performance and scientific reasons, both modes are being implemented using message passing for parallel execution
- Mixed language programming (using C function pointers and wrappers for functional choices)

# Generalized Adaptable Biological Model





# *A Priori* Biological Model



# Example: Use P data to select parameterisations of Z grazing

Table 1. Parameterization of grazing on multiple types of prey with passive selection ( $g_{max}$ : maximum grazing rate; K: Half-saturation constant (but saturation constant in Eq. 1);  $P_0$  threshold below which grazing is zero;  $p_i$ : preference coefficient;  $\alpha, a, \tau$ : constant).

Function	References
(1) Rectilinear $g_i = \begin{cases} g_{\max} \frac{p_i P_i}{K}, & \text{for } R \leq K \\ g_{\max}, & \text{for } R > K \end{cases}, R = \sum_{i=1}^n p_i P_i$	Armstrong, 1994
(2) Ivlev function for each prey type: $g_i = g_{\max} (1 - e^{-\alpha_i P_i})$	Leonard et al., 1999
(3) Ivlev function with interference between prey types: $g_i = g_{\max} (1 - e^{-\alpha R}) \frac{p_i P_i}{R}, \text{ with } R = \sum_{i=1}^n p_i P_i$	Hofmann and Ambler, 1988
(4) Mechanistic disc function: $g_i = g_{\max} \frac{a_i N_i}{1 + \sum_{j=1}^n a_j \tau_j N_j}$	Murdoch and Oaten, 1975; Holt, 1983; Gismervik and Anderson, 1997; Strom and Loukos, 1998
(5) Michaelis Menten Function: $g_i = g_{\max} \frac{p_i P_i}{K + \sum_{j=1}^n p_j P_j}$	Murdoch, 1973; Real, 1977; Moloney and Field, 1991; Verity, 1991; Gismervik and Anderson, 1997; Strom and Loukos, 1998
(6) Threshold MM function: $g_i = g_{\max} \left( \frac{R - P_0}{K + R - P_0} \right) \frac{p_i P_i}{R}, \text{ with } R = \sum_{i=1}^n p_i P_i$	Evans, 1988; Lancelot et al., 2000
(7) Modified MM function: $g_i = g_{\max} \frac{p_i P_i}{1 + \sum_{j=1}^n p_j P_j}$	Verity, 1991; Fasham et al. (1999) and Tian et al. (2001)

Table 2. Parameterization of grazing on multiple types of prey with active switching selection ( $g_{max}$ : maximum grazing rate; K: Half-saturation constant;  $P_0$  threshold below which grazing is zero;  $p_i$ : preference coefficient;  $\alpha, a, \tau$ : constant).

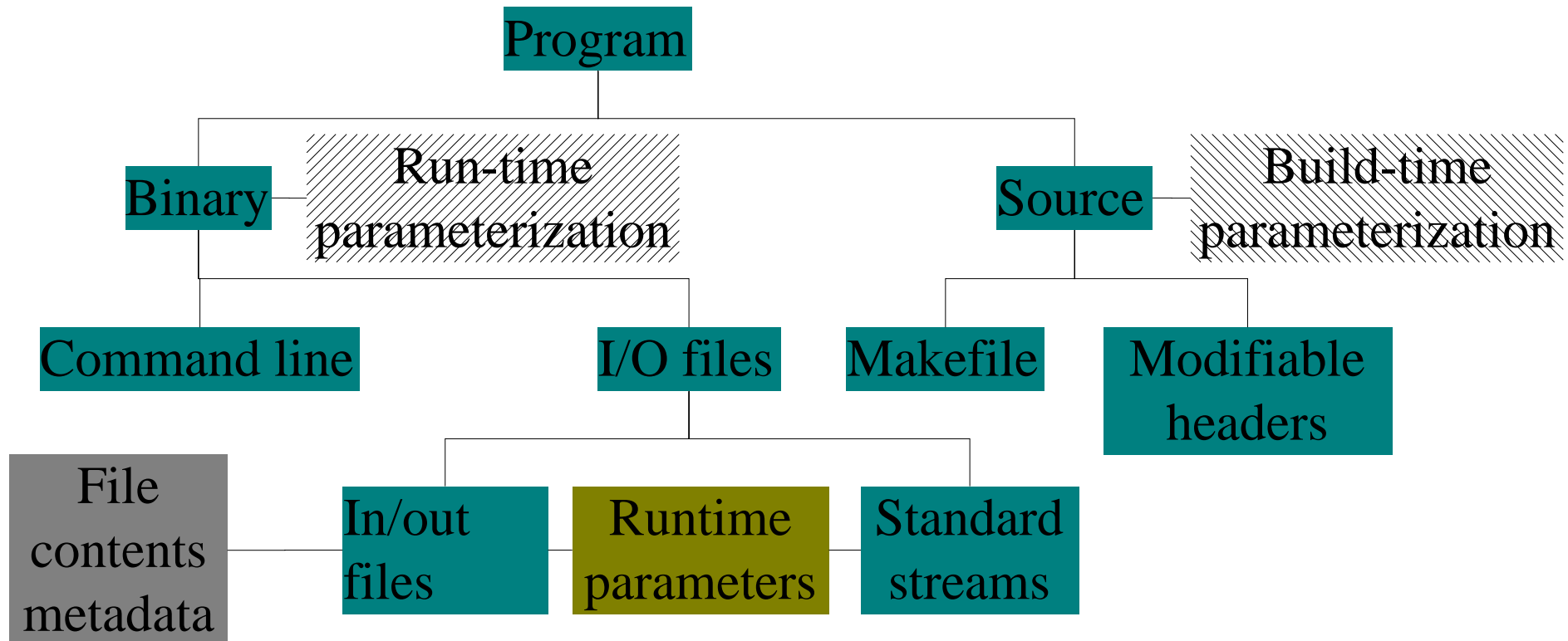
Function	References
(1) Switching MM predation: $g_i = g_{\max} \frac{p_i P_i^2}{K \sum_{j=1}^n p_j P_j + \sum_{j=1}^n p_j P_j^2}$	Fasham et al., 1990; Strom and Loukos, 1998; Pitchford and Brindley, 1999; Spitz et al., 2001
(2) Mechanistic disc switching predation: $g_i = g_{\max} \frac{b_i N_i^2}{(1 + c_i N_i)(1 + \sum_{j=1}^n \frac{b_j h_j N_j^2}{1 + c_j N_j^2})}$	Chesson, 1983
(3) Generalized switching function: $g_i = g_{\max} a_i \frac{(p_i P_i)^m}{\sum_{i=1}^n (p_i P_i)^m}$	Tansky, 1978; Teramoto, 1979; Matsuda et al., 1986
(4) Generalized switching function: $g_i = g_{\max} \frac{(p_i P_i)^m}{\left( \sum_{i=1}^n (p_i P_i) \right)^m}$	Vance, 1978
(5) Generalized switching MM function: $g_i = g_{\max} \frac{(p_i P_i)^m}{1 + \sum_{i=1}^n (p_i P_i)^m}$	Gismervik and Andersen (1997)
(6) Generalized switching MM function: $g_i = g_{\max} \frac{(p_i (P_i - P_{0i}))^m}{1 + \sum_{i=1}^n (p_i (P_i - P_{0i}))^m}$	This work

# Distributed/Grid Computing, Forecasting and Data assimilation with Legacy codes

- Distributed technologies (Sun Grid Engine) with web portal front-end ready to be tested with ESSE and HOPS
- Partial parallelism within ESSE easy because open-source routines (Sun Lapack) were used from the start
- HOPS, ESSE and acoustics codes: Fortran-matlab legacies
  - Relatively complex codes and makefile options
  - Hundreds of build and runtime parameters
- For other (future) codes, source code might not be available
- Classic encapsulation techniques that compartmentalize the code into subroutines, called from wrappers require constant reworking
- Thus: *we chose to encapsulate at the binary level, with generic approach, so as to handle new codes with limited/no rewriting*

# Metadata for handling legacy software

- Hierarchical structure for describing code (can also handle binary-only case)
- Basic assumptions about codes thus encapsulated:
  - No independent GUI, all runtime control from the command line and input/stdin files
  - All build-time parameterization done by altering the makefile and selecting values (parameters) in include-files
- Datatypes and relevant ranges for each parameter checked to ensure validity



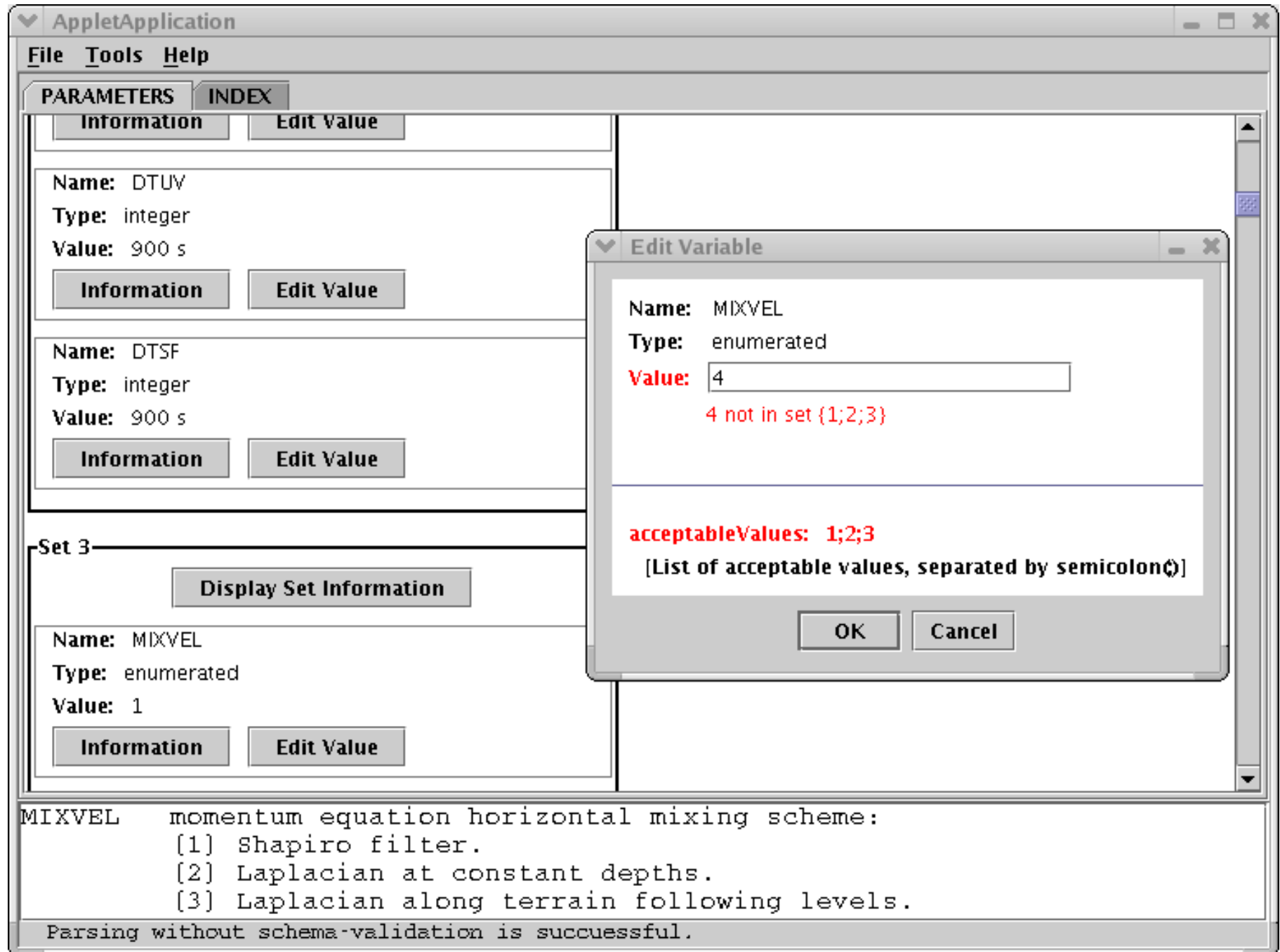
# *XML Encapsulation for Legacy Binaries*

- Descriptions of I/O files, runtime parameters, stdin and command line arguments, makefile parameters, requirements and conflicts for options, invocation mechanisms are needed:
  - Essentially a computer readable install and user guide
  - XML description provides software use and build metadata
  - Design of appropriate hierarchical XML Schemas (evolutionary)
  - Simulation datafile metadata are also usable (e.g. NcML for NetCDF)
  - Provides the constraints for generation of workflows (file I/O based)
- Binaries can be built on demand from generated makefiles
- Developers need to keep XML description up-to-date with their code (incremental effort) without switching to more elaborate approaches
- Concept is generally applicable, directly useful with other ocean models

# Java-Based GUI for Legacy Binaries

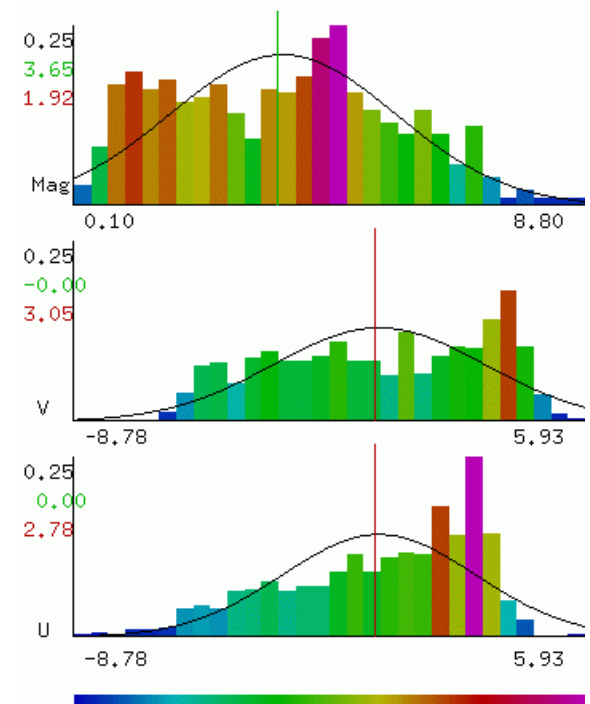
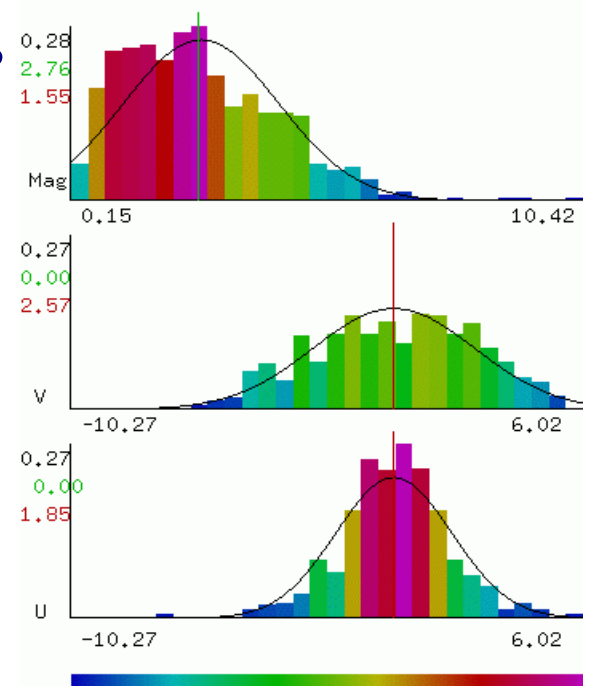
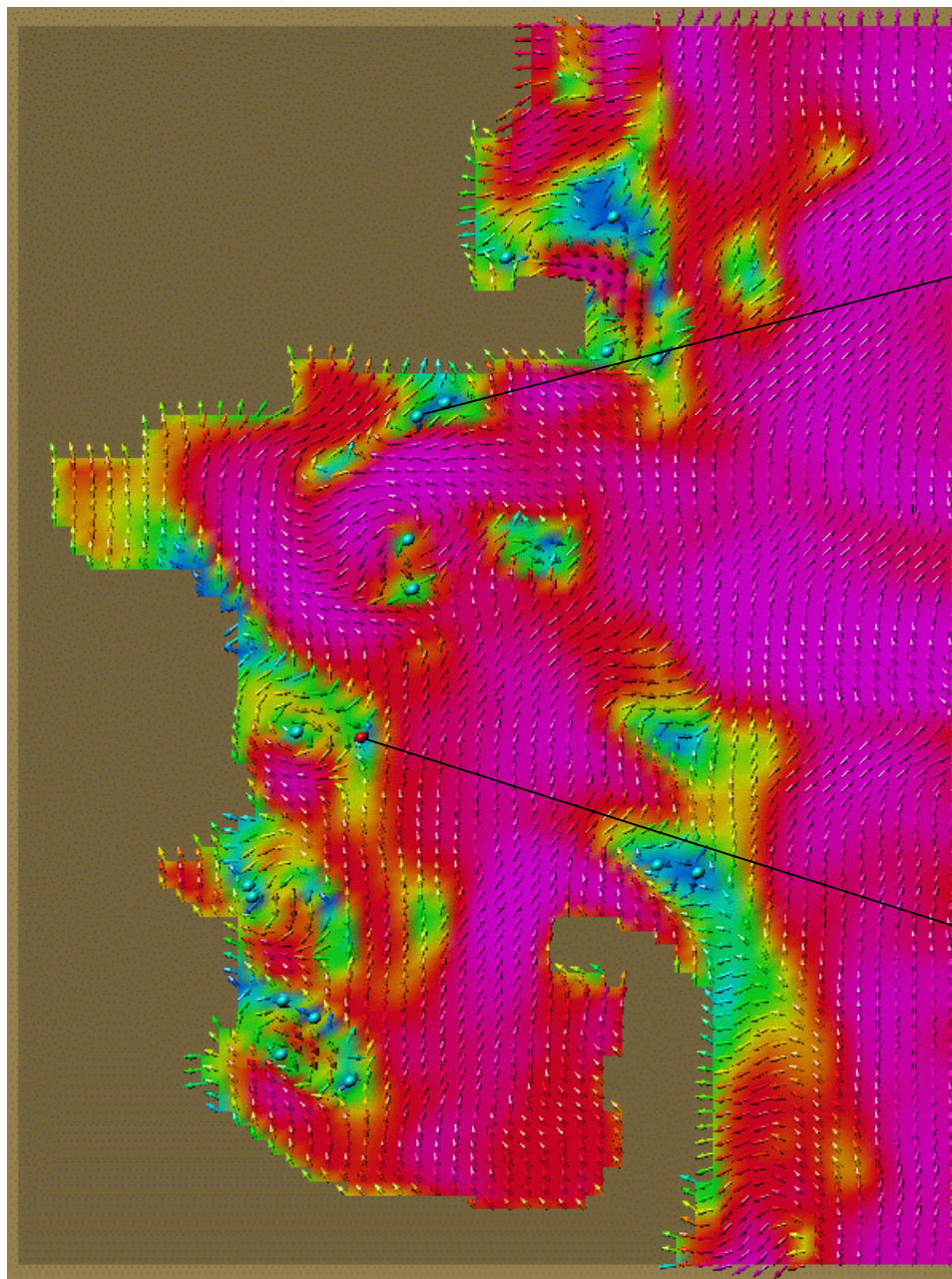
- Prototype GUI, accepts generic set of description files and generates user interface for building and running the binary. Implemented as an applet.
- Validates user choices, generates relevant scripts
- Integral part of the Grid-portal for LOOPS/Poseidon, it can be re-implemented in a more server-centric way (JSP etc.)
- Future directions for enhancement include:
  - Workflow composition: Employing the descriptions of the binaries and their input/output files as constraints. *We are currently using predefined workflows.*
  - Context mediation: When dataflow endpoints mismatch

# GUI: validity checking



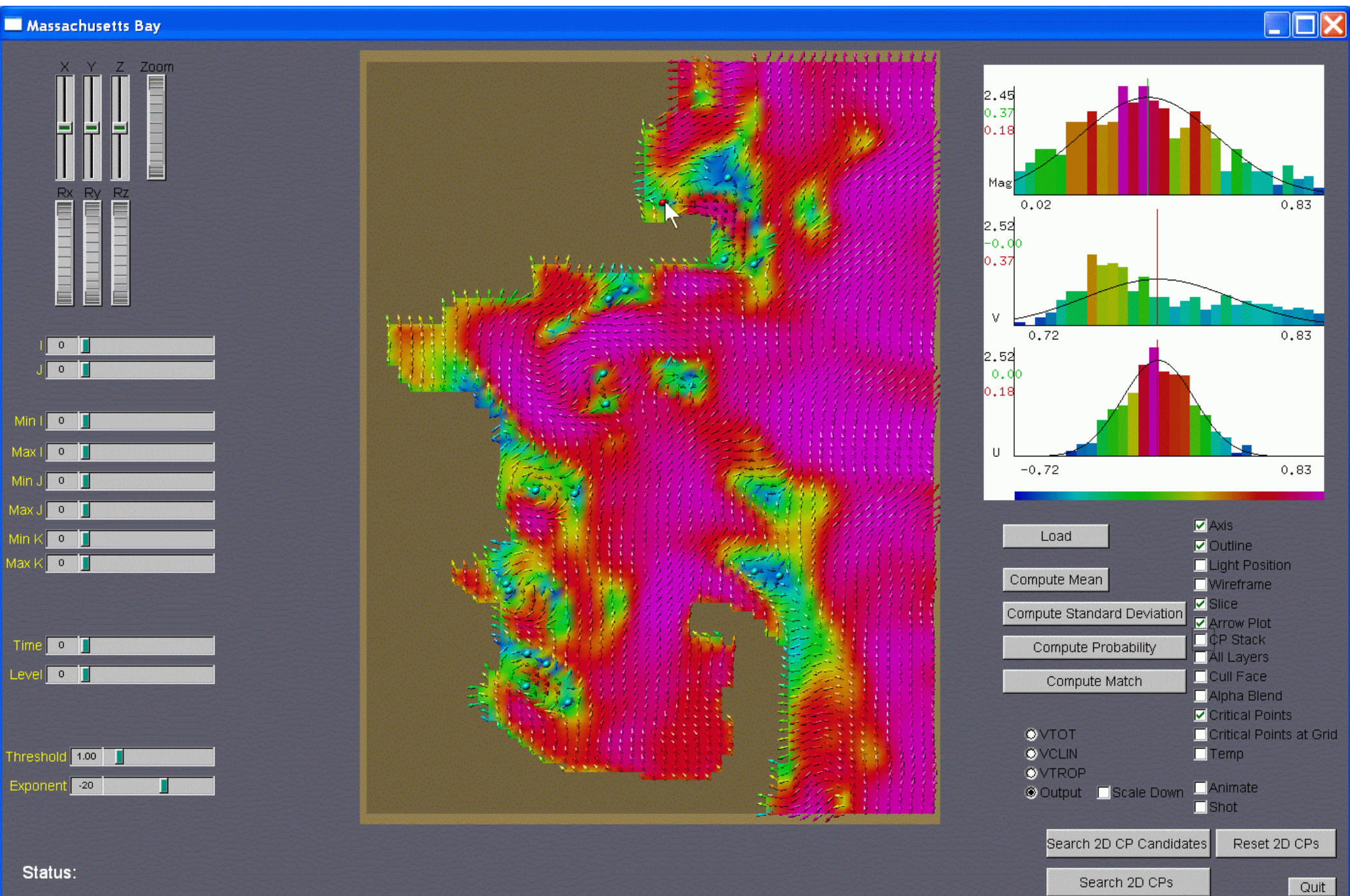


# Interactive Visualization and Targeting of pdf's





# Interactive Visualization and Targeting of pdfs (cont.)



# CONCLUSIONS: Present and Future

- Advanced systems for adaptive sampling and adaptive modeling in a distributed computing environment
- Web interface, Remote visualization, Metadata for code and data, XML-based encapsulation of software, Grid computing infrastructure (SunGridEngine)
- Interdisciplinary data assimilation should contribute significantly to understanding, especially to the quantitative development of fundamental/simplified coupled models
- More interdisciplinary research and education needed: mathematics, computer science, physical-biogeochemical-acoustical ocean science, atmospheric science, earth science and complex system science
- Short-term impacts likely overestimated, long-term effects likely under-estimated



# Feature Extraction for Adaptive Sampling

- Developing automated procedures to identify physical features of interest in the flow: upwelling, eddies & gyres, jets/fronts etc.
- Procedure can be based on a threshold for a derived quantity or a more complicated set of rules.
- Graphical output (in conjunction with uncertainty information) helps the user plan sampling patterns and vehicle paths.

